Directed self-avoiding walks in random media

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Two types of directed self-avoiding walks (SAW's), namely, three-choice directed SAW and outwardly directed SAW, have been studied on infinite percolation clusters on the square lattice in two dimensions. The walks on the percolation clusters are generated via a Monte Carlo technique. The longitudinal extension R_N and the transverse fluctuation W_N have been measured as a function of the number of steps N. Slight swelling is observed in the longitudinal direction on the random lattices. A crossover from shrinking to swelling of the transverse fluctuations is found at a certain length N_c of the walks. The exponents related to the transverse fluctuations are seen to be unchanged in the random media even as the percolation threshold is reached. The scaling function form of the extensions are verified.

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Directed polymers in random environments have versatile applications ranging from growing interfaces to spin glasses to flux lines in high T_c superconductors. The equilibrium properties of linear polymers are well-studied using self-avoiding walk (SAW) models [1]. Properties of SAW's on random lattices have also been studied extensively [2]. Directed polymers are studied using directed SAW models. Two different directed self-avoiding walks (DSAW's), three-choice directed self-avoiding walks (DSAW3's) [3], and outwardly directed self-avoiding walks (ODSAW's) [4,5], are considered here in random media in two dimensions. Figure 1(a) represents the DSAW3, and Fig. 1(b) represents the ODSAW, on the regular square lattice. There is considerable earlier study of DSAW3's [3]. The ODSAW of Fig. 1(b) is less well studied and is imagined to be grown step-by-step such that no step is taken in a direction towards a site already visited. In Fig. 1(b), the step to the site represented by an open circle is not allowed. Hence ODSAW's are ''self-repelling.'' If the origin of the walk is changed from the starting point to the end point, the walk may not satisfy the self-repelling condition [step from X to Y in Fig. 1(b) is not allowed when it starts from the end]. It is then an irreversible walk whereas DSAW's generally are not. DSAW's have a bias of a fixed direction with respect to the embedded space, whereas ODSAW's have a weaker bias of direction with respect to the portion of the SAW already grown. On a regular lattice both DSAW's and ODSAW's can grow indefinitely. The ODSAW's have an additional flexibility in growing, since every DSAW is a ODSAW. In this paper, the effect of randomness of the medium on these directed walks is studied.

It is believed that a change in universality occurs for the ordinary SAW's at strong disorder [2,6]. Directed SAW's are more restricted than ordinary SAW's in general. It is then interesting to study the effect of randomness of the medium on directed SAW's. Kardar and Zhang [7] have indirectly shown for the transverse fluctuation of the minimum-energy paths on random energy landscapes that there is a change in the scaling exponent from 1/2 to 2/3 in the zero-temperature and strong-disorder limit. In a similar model, Cook and Derrida [8] performing a $1/d$ expansion and n-tree approximation, were unable to find such a transition. Monte Carlo results of two directed SAW's, described above, on infinite percolation clusters, are presented here for the first time. No change in exponent due to randomness of the lattice is observed. A slight swelling in the longitudinal direction and a crossover from shrinking to swelling in the transverse fluctuation after certain steps of the walks are observed. The scaling function form of the extensions are tested through data collapse. The longitudinal extension scaling function is similar to that of the extension of ordinary SAW's on random lattices.

There are two stages of the simulation. First, percolation clusters for different p values, including the percolation threshold $p_c \approx 0.593$, have been generated on the square lattice of size $2^{10} \times 2^{10}$. The single cluster growth method [9] is used to generate percolation clusters from the central site of the lattice. Only the infinite or spanning clusters that connect all opposite boundaries of the lattice are considered. Second, the walks are generated as described in Fig. 1 on those infinite percolation clusters using a Monte Carlo (MC) technique. In a MC step in generating a walk, the number n_s of possible open paths is calculated for the next step and a step is selected with a probability $1/n_s$. Both the longitudinal extension R_N and transverse fluctuation W_N of the walks have been measured with the number of steps N (length) of the walks on random ($p<1$) and regular ($p=1$) lattices. In general, the quantities R_N and W_N are given by

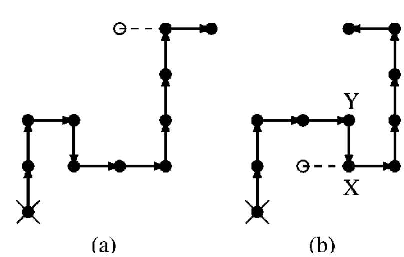

FIG. 1. DSAW3 (a) and ODSAW (b) on a regular square lattice. The ODSAW can not have any step towards itself. The step towards the sites represented by an open circle in both (a) and (b) are forbidden. If the ODSAW starts from the end then the step X to Y is also forbidden.

$$R_N(p) \approx A(p) N^{\nu_\parallel(p)}, \quad W_N(p) \approx B(p) N^{\nu_\perp(p)}, \tag{1}$$

where $\nu_\parallel$ and $\nu_\perp$ are the corresponding exponents and $A(p)$ and $B(p)$ are the amplitudes.

In generating a walk starting from a randomly chosen origin, periodic boundary conditions are applied in both directions if the walk hits the boundary of the lattice. On the regular ($p=1$) square lattice 10^4 walks of $N=10^6$ steps are generated. As randomness is introduced into the medium the indefinitely growing walks will be terminated because of the irregularity of the medium. This may happen for two reasons. First, a walk may terminate by hitting the dangling ends at the outer boundary of a random cluster. Second, the percolation clusters contain self-similar blobs connected by narrow necks [10] and the SAW's may be confined or partially localized in such blobs as the randomness of the cluster increases. To incorporate proper configurational averages more and more random clusters $C(p)$ are generated as p is decreased from 0.9 to the percolation threshold $p_c \approx 0.593$. The values of $C(p)=200$ for $p=0.9$, $C(p)=400$ for $p=0.8$, $C(p)=800$ for $p=0.7$, and $C(p)=1600$ for $p=p_c \approx 0.593$ are chosen. On each configuration 100 different walks are attempted from randomly chosen origins including the central site from which the cluster is grown. In total $100\times C(p)$ walks are then grown for a particular value of p. Not all the walks perform the same number of steps on a random lattice. Counts of the number of walks $n_w(N)$ performed up to N steps are kept and the averages are made accordingly.

To measure the longitudinal extension R_N and the transverse fluctuation W_N of the walks on the regular and random lattices, the radius of gyration tensor $\mathbf{T}$ is calculated. For an N-step walk the ijth component of the tensor is given by

$$T_{ij}(N) = \frac{1}{N+1} \sum_{l=1}^{N+1} (x_{li} - \langle x_i \rangle)(x_{lj} - \langle x_j \rangle), \tag{2}$$

where the lth site is located at $\mathbf{x}_l$ (N-step walks has $N+1$ sites). The quantity x_{li} is the ith component of $\mathbf{x}_l$ and $\langle x_i \rangle$ is the ith component of the center of mass position $\langle \mathbf{x}_l \rangle = \sum_{l=1}^{N+1} \mathbf{x}_l/(N+1)$. The root-mean-square values of R_N and W_N can be calculated from the large λ_L and small λ_S eigenvalues of the radius of gyration tensor $\mathbf{T}$, a 2×2 matrix here. The extensions are then $R_N = \sum_{k=1}^{n_w} \lambda_{Lk}/n_w$ and $W_N = \sum_{k=1}^{n_w} \lambda_{Sk}/n_w$. Note that n_w on the regular lattice is arranged to be 10^4 regardless of N.

Since both amplitude and exponent of the extensions in Eq. 1 are functions of p (the randomness of the medium), it is then interesting to see how they are modified in random media. First, the scaling exponents related to the longitudinal and transverse extensions are considered. The value of the longitudinal extension exponents for both the walks are known, i.e., $\nu_\parallel = 1$ on the regular lattice. For DSAW3's, this may be found in Ref. [3]. For ODSAW's, it is obtained through MC simulation by Turban and Debierre [4], and it is also recently tested through exact enumeration by Santra *et al.* [5]. The transverse fluctuation exponent is $\nu_\perp = 1/2$ for DSAW3's [3] on the regular lattice, so that DSAW3's are anisotropic in nature. But the ODSAW's treat all lattice directions equivalently and therefore are isotropic. Thus for ODSAW's on the regular lattice, the value of the exponent $\nu_\perp$ should also be 1 in the asymptotic limit $N\to\infty$. In the numerical simulation for ODSAW's of 10^6 steps, $\nu_\perp$ is found ≈ 0.97, which is close to the expected value of 1. Since the exponent $\nu_\perp$ of ODSAW's is different from that of DSAW3's, the ODSAW's then belong to a new universality class. It is expected that the value of the exponents should increase when the walks are performed in the random medium. Since the value of $\nu_\parallel$ of both the walks and $\nu_\perp$ of ODSAW's are already equal to 1 on the regular lattice, there is then no scope for increase the value of these exponents of the directed walks considered here in random media. Only the exponent $\nu_\perp$ of DSAW3's could increase due to the randomness of the medium. In Fig. 2, W_N for DSAW3's is plotted against N, the number of steps, for different values of p to see how the disorder modifies the exponent $\nu_\perp$. Data up to N steps are considered in this plot (for $p<1$) such that at least 10^3 walks have been sampled. The data for the regular lattice (circles) verify the scaling relation given in Eq. (1). For DSAW3's, $\nu_\perp$ is found 1/2 as expected. Intriguingly it is seen that the data for different p values ($p=0.9$ to $p=p_c \approx 0.593$) follow the same curve as that of the $p=1$ regular lattice. Though the data for $p<1$ remains in the part of the plots displaying curvature, the exponent $\nu_\perp$ for the DSAW3's seems to be the same for any value of p. So the universality, as well as the critical properties of the walk, remain unchanged even as the percolation threshold is approached. This is an important observation and very different from the results obtained by Kardar and Zhang [7], whose model is, however, somewhat different. Kardar and Zhang considered the minimum-energy paths and not the zero energy paths on a landscape where the bond energies parallel to the time axis are random and occupation of the perpendicular bonds costs a constant energy. The walks considered in our

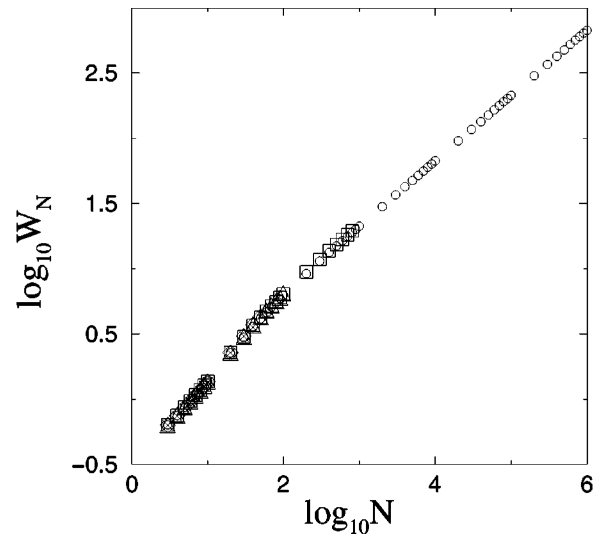

FIG. 2. Plot of transverse fluctuation W_N of DSAW3's versus N, the number of steps, for different values of p. Different symbols are (○) for $p=1$, (□) for $p=0.9$, (△) for $p=0.8$, (◇) for $p=0.7$, and (×) for $p=0.593$.

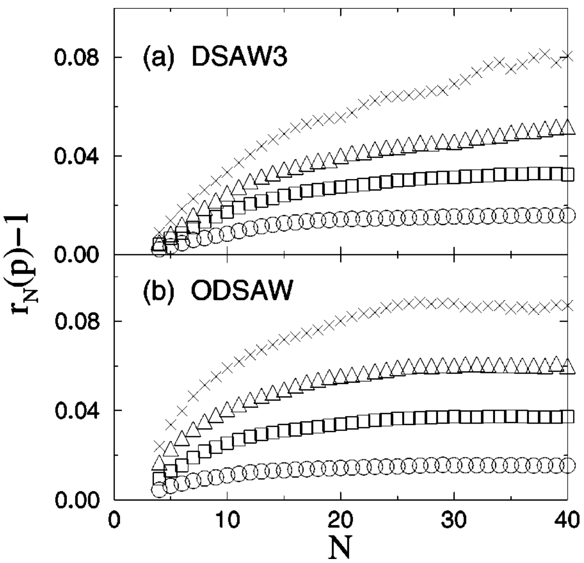

FIG. 3. Plot of $\omega_N(p)-1$ for (a) DSAW3's and (b) ODSAW's versus number of steps N. Symbols are (○) for $p=0.9$, (□) for $p=0.8$, (△) for $p=0.7$, and (×) for $p=0.593$. There is a crossover from shrinking to swelling.

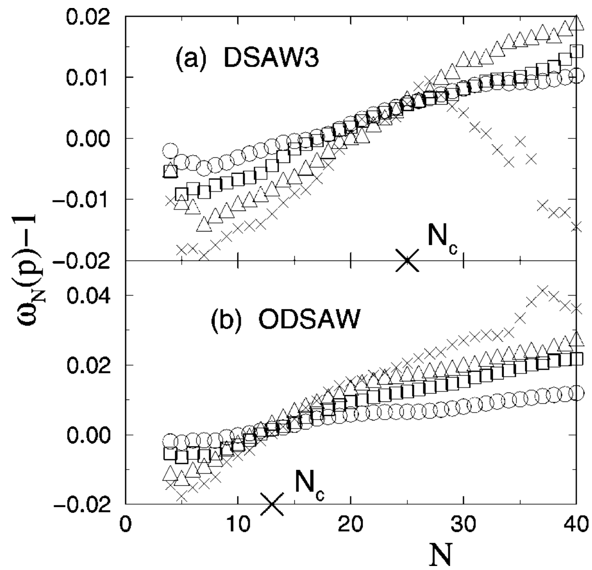

FIG. 4. Plot of $R_N(p)/R_N(p_c)$ for (a) DSAW3's and (b) ODSAW's versus the scaled variable $N(p-p_c)^{\zeta_p}$ up to $N=25$ steps. The value of ζ_p is taken 1.68. The symbols are: (○) for $p=1$, (□) for $p=0.9$, (◇) for $p=0.8$, and (△) for $p=0.7$.

model are of zero energy. The associated energy with the empty sites of the percolation cluster is infinite and they are forbidden for the walker. In our model, all the possible walks from a point A to a point B may be forbidden due to the randomness of the lattice whereas in the Kardar and Zhang model there will be always a minimum-energy path connecting A and B. The results obtained by Kardar and Zhang may be related to the particular model they have considered in connection to the domain wall boundary of the Ising spin systems at zero temperature [11].

Next, the variation of the amplitudes $A(p)$ and $B(p)$ are considered in random media. Generally the amplitude of ordinary SAW's increases or they swell in random media [2] but it is not known how amplitudes of directed SAW's behave in random media. To understand the variation of the amplitudes of DSAW3's and ODSAW's in random media, a measure is defined as the ratio of the amplitudes for $p<1$ to that of $p=1$. Since the exponents ν related to R_N and W_N are independent of p, the ratios of the amplitudes are then $r_N=A(p<1)/A(p=1)=R_N(p<1)/R_N(p=1)$ for R_N and $\omega_N=B(p<1)/B(p=1)=W_N(p<1)/W_N(p=1)$ for W_N. In Fig. 3 the ratio $r_N(p)$ is plotted against the number of steps N for both the walks. It is observed that $r_N(p)>1$ always for any length N of the walks. There is then swelling of the longitudinal extension R_N of these directed walks on the random lattices for all possible lengths of the walks. However the swelling found is small, for strong disorder (at $p=p_c$) $\approx 8\%$ to 9%. The ratio $\omega_N(p)$ of the transverse fluctuations is plotted against N in Fig. 4. Initially $\omega_N(p)$ is less than 1, but it increases with the length N and becomes greater than 1 for long walks. For both the walks, there is then a crossover from shrinking to swelling at a certain length of the walks. This is a new and interesting result. For DSAW3's the crossover is around 25 steps and in the case of ODSAW's, it is around 13 steps. Thus there exists a crossover length N_c of the directed walks below which the swelling of the longitudinal extension partially comes from the shrinking in the transverse direction in a random medium. Since the percolation cluster contains self-similar blobs connected by narrow links, these short walks are confined either in those narrow links or within the blobs of size smaller than that crossover length N_c. One important length scale of the node-link-blob model [12,10] of the percolation clusters is involved here. That is the distance between two nodes or the chemical distance L_l. If a walk is shorter than L_l, then the walk will feel the fractal nature of the percolation cluster strongly. As a consequence, a directed walk, elongated in a particular direction, will have less freedom in growing in a transverse direction. But a long walk, longer than L_l as well as the correlation length (shortest distance between the nodes), could diffuse over several blobs and swell in both directions. Note that the crossover length N_c of two directed walks are different. This means that the diffusion of the directed walks on random lattices depends not only on the shape of the random cluster but also on the nature of the directed walks. A shorter walk of the highly flexible ODSAW's than a walk of the more restricted DSAW3's could always find a path to diffuse from blob to blob. The drop of $\omega_N(p)$ at p_c for longer lengths is possibly due to poor sampling. Only 806 DSAW3's and 1742 ODSAW's survive up to 40 steps out of 16×10^4 walks. Note that the swelling of ODSAW's in both the directions are higher than that of DSAW3's because of their high flexibility.

Finally, the scaling function forms of R_N and W_N with $(p-p_c)$ is verified. The chemical distance scales as $L_l\sim(p-p_c)^{-\zeta_p}$ with an exponent ζ_p. Numerically the value of ζ_p is obtained as 1.68 in two dimensions [13]. Hence, the longitudinal extension R_N of the walks on random lattices should follow a scaling form

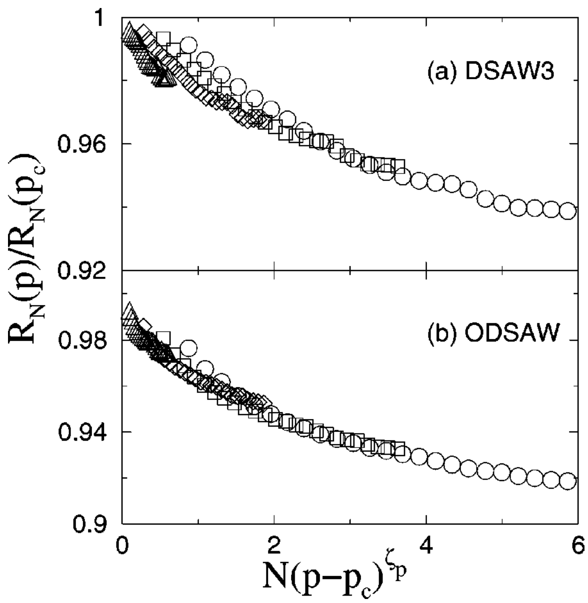

FIG. 5. Plot of $R_N(p)/_N(p_c)$ for (*a*) DSAW3s and (*b*) ODSAWs versus the scaled variagle $N(p-p_c)^{\zeta_p}$ up to $N=25$ steps. The value of ζ_p is taken 1.68. The symbols are: circles for $p=1$, boxes for $p=0.9$, jdiamonds for $p=0.8$ and triangles for $p=0.7$. A reasonable data collapse is observed for both the walks.

$$R_N \sim N^{\nu_\parallel} \mathsf{f}_R(N(p-p_c)^{\zeta_p}), \tag{3}$$

where the scaled variable is $N/L_l = N(p-p_c)^{\zeta_p}$. In Fig. 5, $R_N(p)/R_N(p_c)$ is plotted against the scaled variable $N(p-p_c)^{\zeta_p}$ up to $N=25$ steps. It is expected that the data $R_N(p)/R_N(p_c)$ should collapse on to a single curve f_R for any value of N/L_l if $\mathsf{f}_R(0)$ is a constant. First, note that f_R approaches 1 as the scaled variable $N(p-p_c)^{\zeta_p}$ approaches 0. Second, a reasonable collapse of data is observed for both the walks, especially for ODSAW's. The longitudinal extension R_N then follows the scaling function form given in Eq. (3). Note that the data collapse should occur within the critical regime of the percolation threshold. But here data for a wide range of $(p-p_c)$ have been considered. The extension of the ordinary SAW's on random lattices follows the same scaling function form [2,14]. To find the scaling function form for the transverse fluctuation W_N of the directed walks on random lattices one needs to introduce another length scale on the percolation cluster. This new length L_t must be perpendicular to the chemical distance L_l and could be considered as the cross section of the links. In two dimensions it is reasonable to assume that $L_t L_l$ is constant. The transverse length L_t then scales as $L_t \sim (p-p_c)^{\eta_p}$, where $\eta_p = \zeta_p$. The existence of the crossover length N_c can also be understood in terms of the transverse length L_t. As $p \to p_c$, L_t tends to zero, i.e., the links are connected by single bonds. In this regime the shorter walks are typically confined within the isolated blobs or in the narrow necks. A scaling form of W_N thus can be written as $W_N \sim N^{\nu_\perp} \mathsf{f}_W((p-p_c)^{\eta_p}/N)$ where the scaled variable is L_t/N. The behavior of $W_N(p)/W_N(p_c)$ is studied as a function of the scaled variable L_t/N for $\eta_p = \zeta_p = 1.68$ and also for other different values of η_p. But no collapse of data on to a single curve f_W is found for a wide range of η_p. This may be due to an incorrect scaling form assumed for the transverse length L_t or due to an important correction to scaling. To resolve this, one could study the scaling of L_t with $(p-p_c)$ on the percolation cluster itself.

In summary, the longitudinal extension R_N and the transverse fluctuation W_N of two directed self-avoiding walks, DSAW3's and ODSAW's, on random lattices in two dimensions have been studied. There is some swelling of the longitudinal extension R_N on the random lattices. The transverse fluctuations W_N show a crossover from shrinking to swelling at a certain length N_c of the walks. The exponent $\nu_\perp = 1/2$ for DSAW3's seems to be independent of the randomness (p) of the lattice. There is then no change in the scaling exponents in random media except a little swelling or shrinking in their size depending on the length of the walks. The scaling function form of the longitudinal extension of these directed SAW's is verified and it is similar to that of the ordinary SAW's on random lattices.

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